Risk Assessment for Nanomaterials: Emerging Tools and Value of Information Analysis

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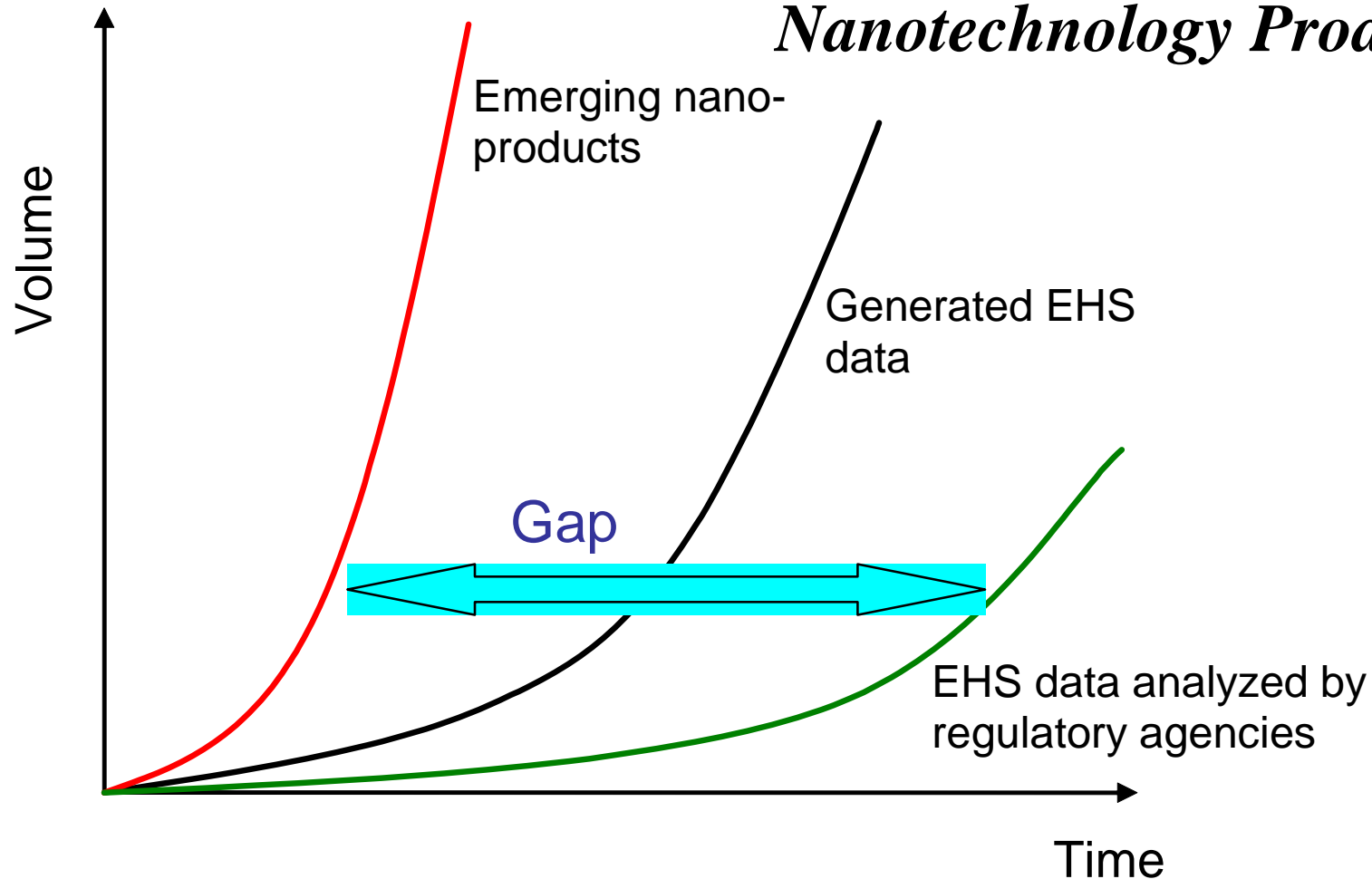Igor.Linkov@usace.army.mil, Phone: 6172339869

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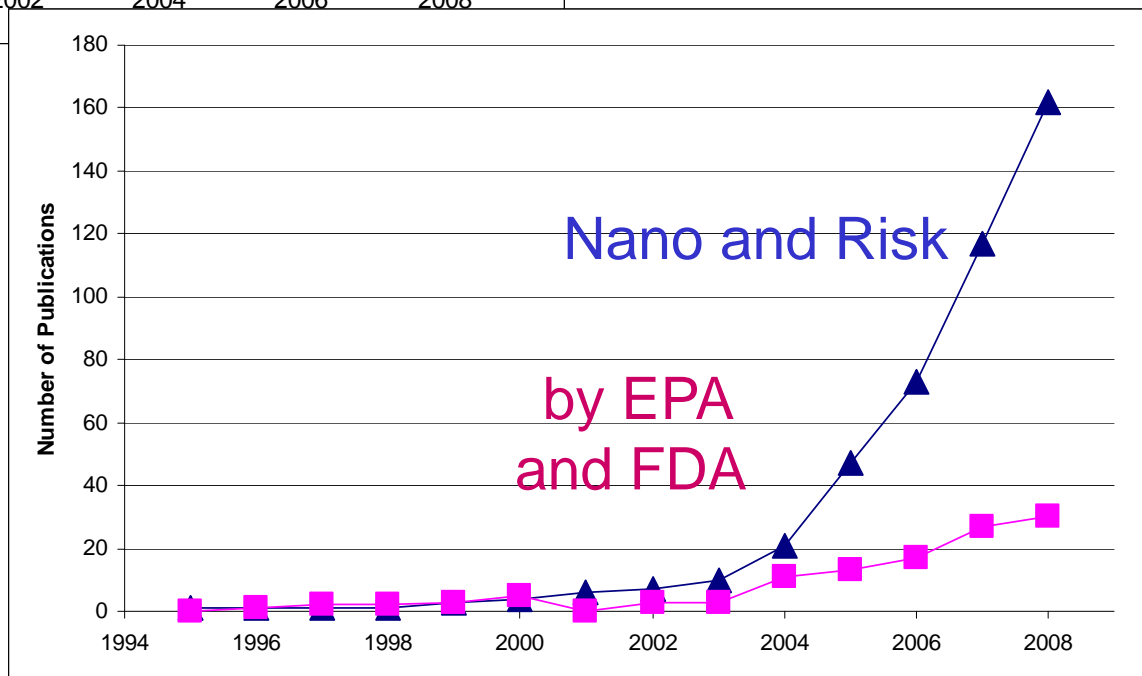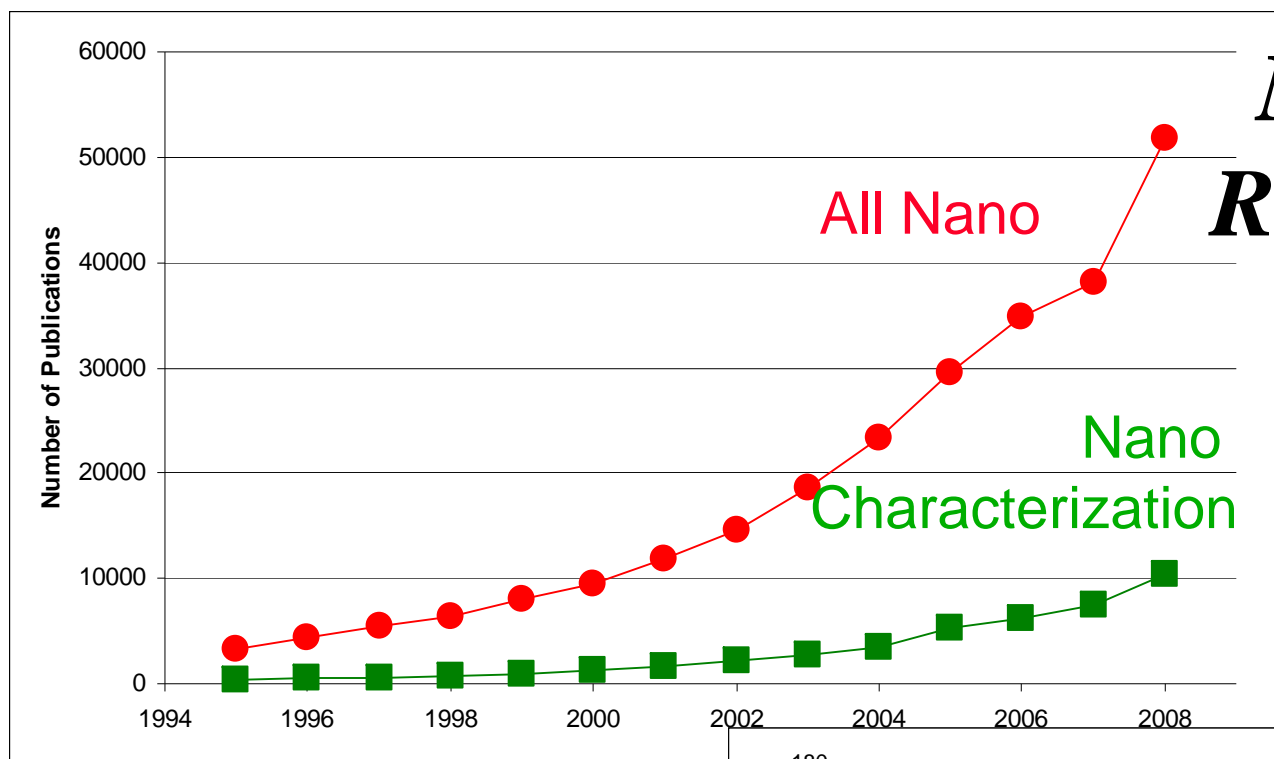| 16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
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Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

Problem: Nano EHS Data for Risk Assessment is Insufficient Because of Fast Emergence of Nanotechnology Products

Volume

Emerging nano-products

Generated EHS data

Gap

EHS data analyzed by regulatory agencies

Time

Increasing gap requires innovative risk management

Nanotech and Risk Assessment Published Papers

All Nano

Nano Characterization

Nano and Risk

by EPA and FDA

After Linkov et al., 2009

- Relation of pattern, structure-activity and physico-chemical properties of nanoparticles on toxicity and life-cycle risk is widely unknown and available information is fragmented.

- Challenges of risk assessment and management for situations with a limited knowledge base and high uncertainty and variability require coupling traditional risk assessment with multi-criteria decision analysis (MCDA) and Life Cycle Assessment (LCA) to support sustainable nanomanufacturing and regulatory decision making.

- Entities engaged in nanotech must consider practical and innovative steps to develop sustainable nanomaterials minimizing identified life-cycle product risk while keeping costs down.
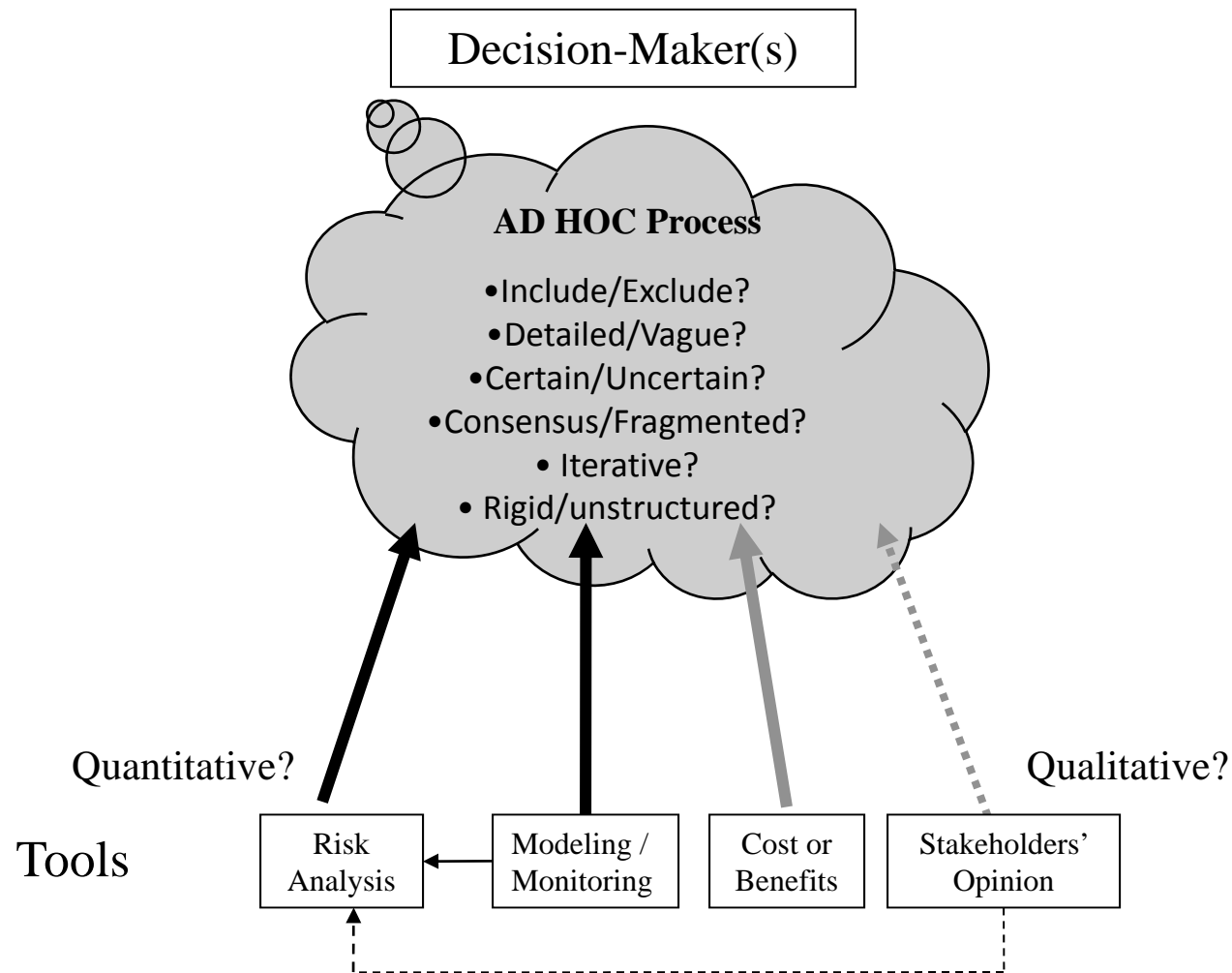
- Intro to Multi-Criteria Decision Analysis

- Nano and Traditional Risk Assessment

- Integration of RA/MCDA/LCA for Nano: Carbon Nanotubes Manufacturing Case Study
  - Problem
  - LCA assessment
  - Integrated RA/MCDA
  - Incorporation of Stakeholder Preferences
  - Value of Perfect Information Analysis
  - Value of Imperfect Information Analysis

- Conclusions

Decision-Maker(s)

AD HOC Process

•Include/Exclude?
•Detailed/Vague?
•Certain/Uncertain?
•Consensus/Fragmented?
• Iterative?
• Rigid/unstructured?

Quantitative?

Qualitative?

Tools

| Risk Analysis | Modeling / Monitoring | Cost or Benefits | Stakeholders' Opinion |

Challenge: Multiple & Uncertain Criteria

Problem: Parameter Uncertainty

- Parameter Uncertainty

- Uncertainty and variability in
  model parameters resulting from
  – data availability
  – expert judgment
  – empirical distributions

- Can be addressed by
  – Probabilistic Simulations (Monte-Carlo)
  – Analytical techniques (uncertainty propagation)
 – Expert estimates
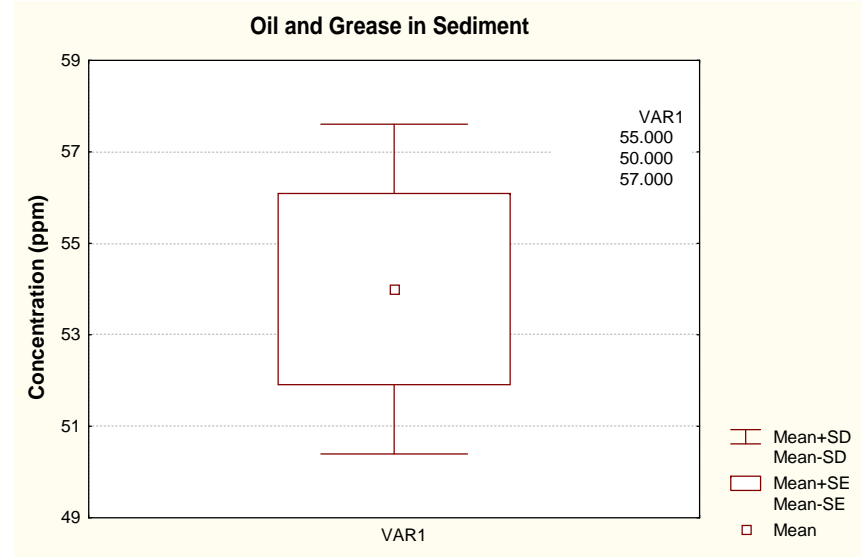
Many parameters and factors important for risk assessment are not well known, reported ranges are large and often unquantifiable

Oil and Grease in Sediment

VAR1
55.000
50.000
57.000

Concentration (ppm)

VAR1

Mean+SD
Mean-SD
Mean+SE
Mean-SE
Mean

Problem: Model Uncertainty

- ▪ Model Uncertainty
  - – Differences in model structure resulting from:
    - ◆ model objectives
    - ◆ computational capabilities
    - ◆ data availability
    - ◆ knowledge and technical expertise of the group
  - – Can be addressed by
    - ◆ considering alternative model structures
    - ◆ weighting and combining models
    - ◆ Eliciting expert judgment
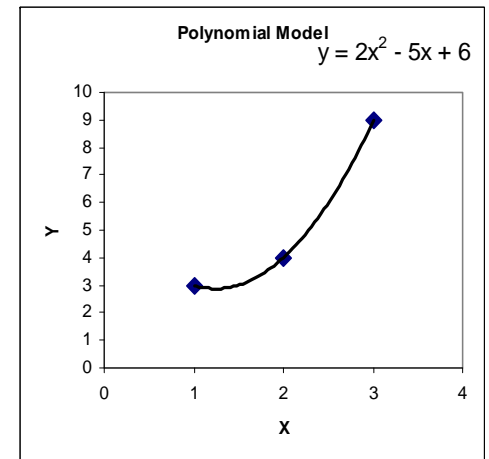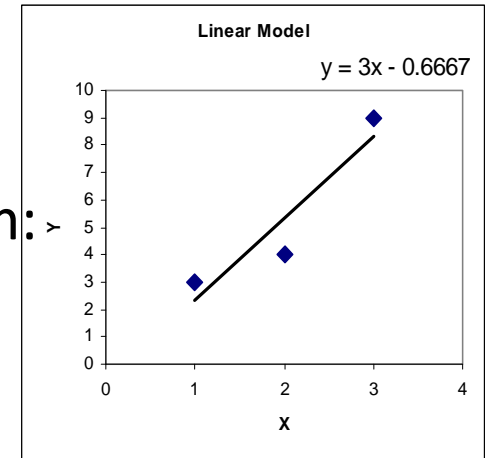
Mechanistic models for environmental risk assessment are very uncertain and expert judgment is required

Linear Model

$y = 3x - 0.6667$

Polynomial Model

$y = 2x^2 - 5x + 6$

subjective interpretation of the problem at hand

WHAT DO YOU SEE ?

A HAT

OR

A BOA CONSTRICTOR

DIGESTING AN ELEPHANT

What is the relative influence of modeler perception on model predictions?

After Antoine Marie Roger de Saint-Exupéry

Multi-Criteria Decision Analysis

- Refers to a group of methods used to impart structure to the decision-making process

- Generally consists of four steps:
  - Creating a hierarchy of criteria relevant to the decision at hand, for use in evaluating the decision alternatives
  - Weighting the relative importance of the criteria
  - Scoring how well each alternative performs on each criteria
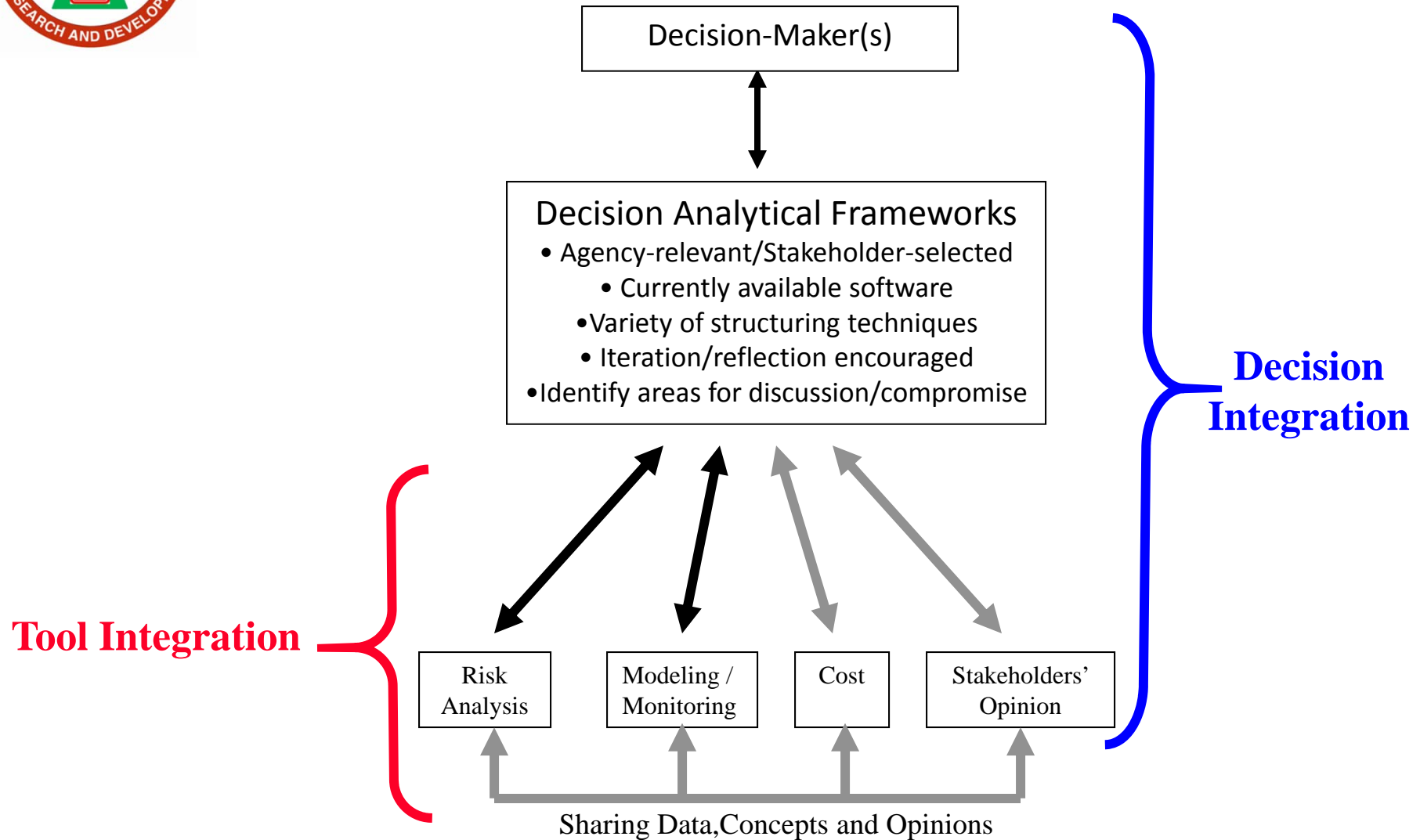 - Combining scores across criteria to produce an aggregate score for each alternative

Multi-Criteria Decision Analysis and Tools

- Multi-Criteria Decision Analysis (MCDA) methods:
  - Evolved as a response to the observed inability of people to effectively analyze multiple streams of dissimilar information
  - Many different MCDA approaches based on different theoretical foundations (or combinations)

- MCDA methods provide a means of integrating various **inputs** with stakeholder/technical expert **values**

- MCDA methods provide a means of communicating model/monitoring **outputs** for regulation, planning and stakeholder understanding

- **Risk-based MCDA** offers an approach for organizing and integrating varied types of information to perform rankings and to better inform decisions

Evolving Decision-Making Processes

Decision-Maker(s)

Decision Analytical Frameworks
- Agency-relevant/Stakeholder-selected
- Currently available software
- Variety of structuring techniques
- Iteration/reflection encouraged
- Identify areas for discussion/compromise

Decision Integration

Tool Integration

| Risk Analysis | Modeling / Monitoring | Cost | Stakeholders' Opinion |

Sharing Data, Concepts and Opinions

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Simplified Decision Matrix

Plan	Cost	Eco Health	Human Health
A	100	10	5
B	100	5	10
C	150	10	10
D	150	10	15

Example Decision Matrix

How to combine these criteria?

		Criteria 1	Criteria 2	Criteria 3	Criteria 4
Alt. 1					
Alt. 2		Monitoring Results	Stakeholder Preference	Economic Cost	Non-monetary benefit
Alt. 3		Mo...lts	Stakeholder Preference	Economic Cost	Non-monetary benefit
Alt. 4		Mo...lts	Stakeholder Preference	...st	Non-monetary benefit

How to interpret these results?

How to compare these alternatives?

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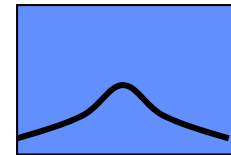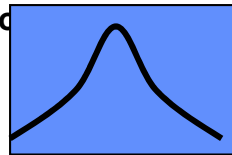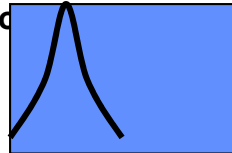
Risk Assessment Formulation

What can happen (go wrong)?

How likely is it?

Kaplan & Garrick 1981

What are the consequences?
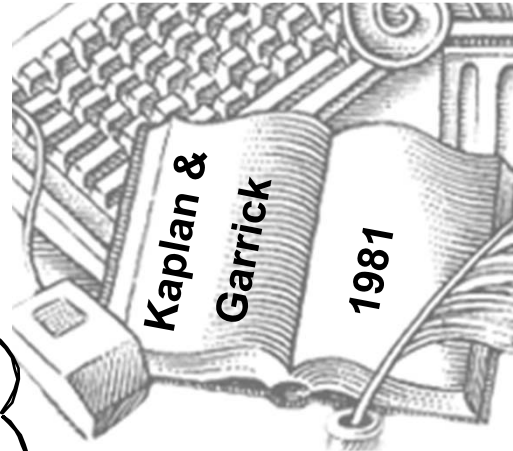
- Goal: Will exposure to a contaminant cause adverse health effects?

- Based on data (often limited and imprecise) regarding toxic effects of materials on people and animals

- State-of-the-science risk assessment is not very far advanced
  - Two general bodies of data
    - Toxicity studies in animals
    - Epidemiologic studies in humans
  - Uncertainties can be tremendously large

- Often handled as a "bright line" approach, but typically plagued with uncertainties

Benchmarks – Reflection of "Acceptable" Risk

$$HQ = \frac{MediaConcentration}{Benchmark}$$

**Hazard Quotient
(Chemical-Specific)**

$$HI = \sum_i HQ_i$$

**Hazard Index
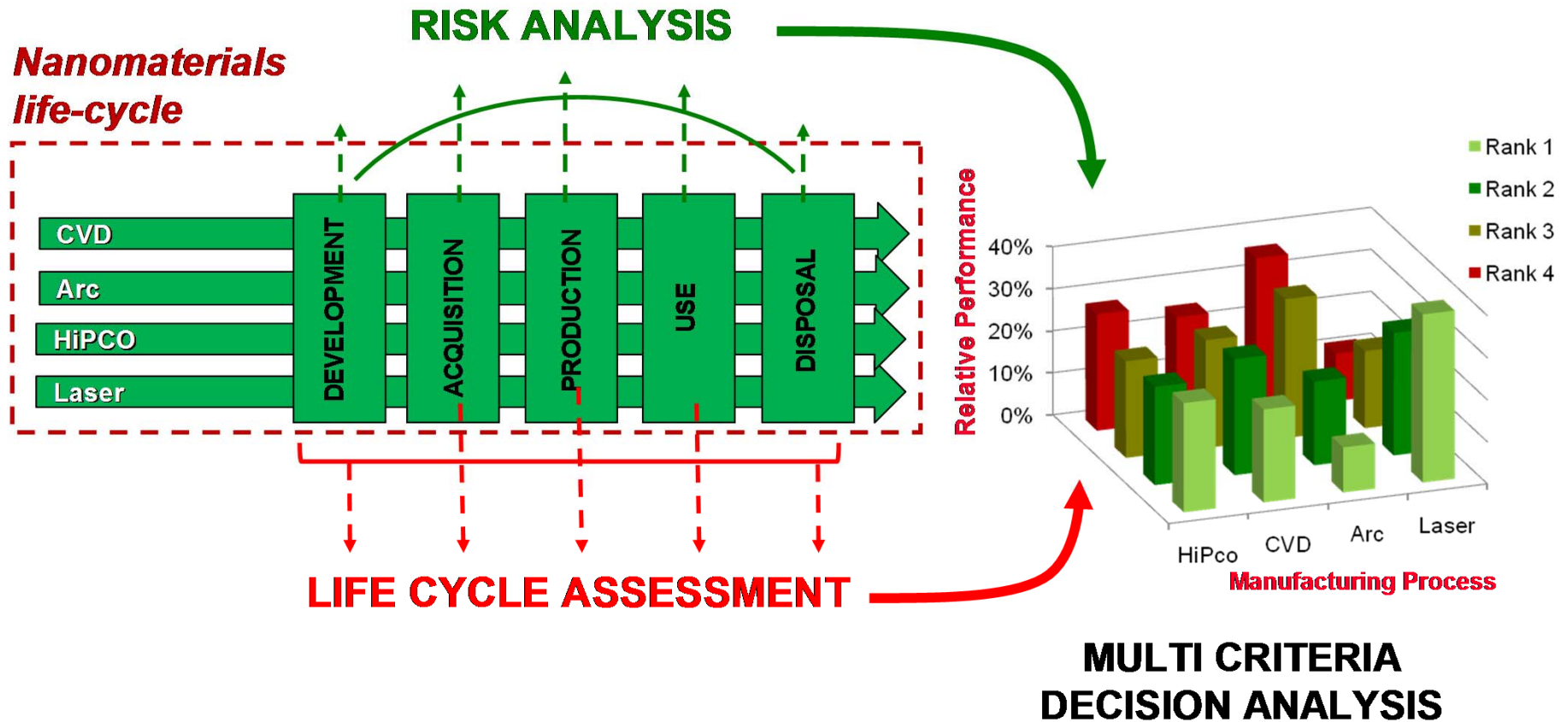(Cumulative)**

No benchmarks for nano!

- Problem: find optimal manufacturing process for SWCNT (Single Wall Carbon Nano Tubes)

- Consideration of 4 manufacturing process alternatives: HiPco, Arc, Laser, CVD

- Combined MCDA (stochastic version of PROMETHEE II) on energy and material efficiency, life cycle score, health risk and cost

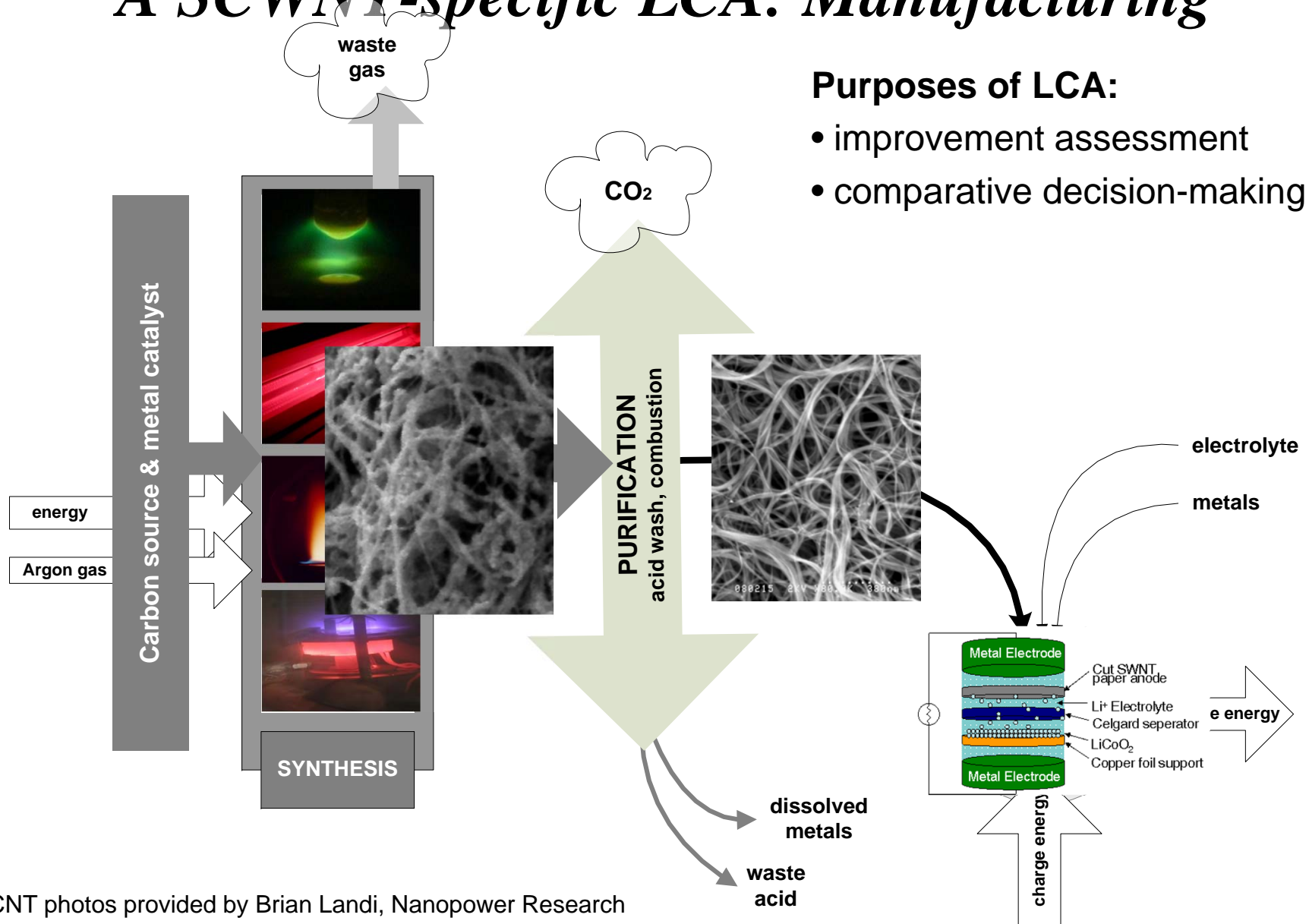After Seager and Linkov, 2008, and
Canis, Seager, Linkov, 2010

Linking RA, LCA and MCDA

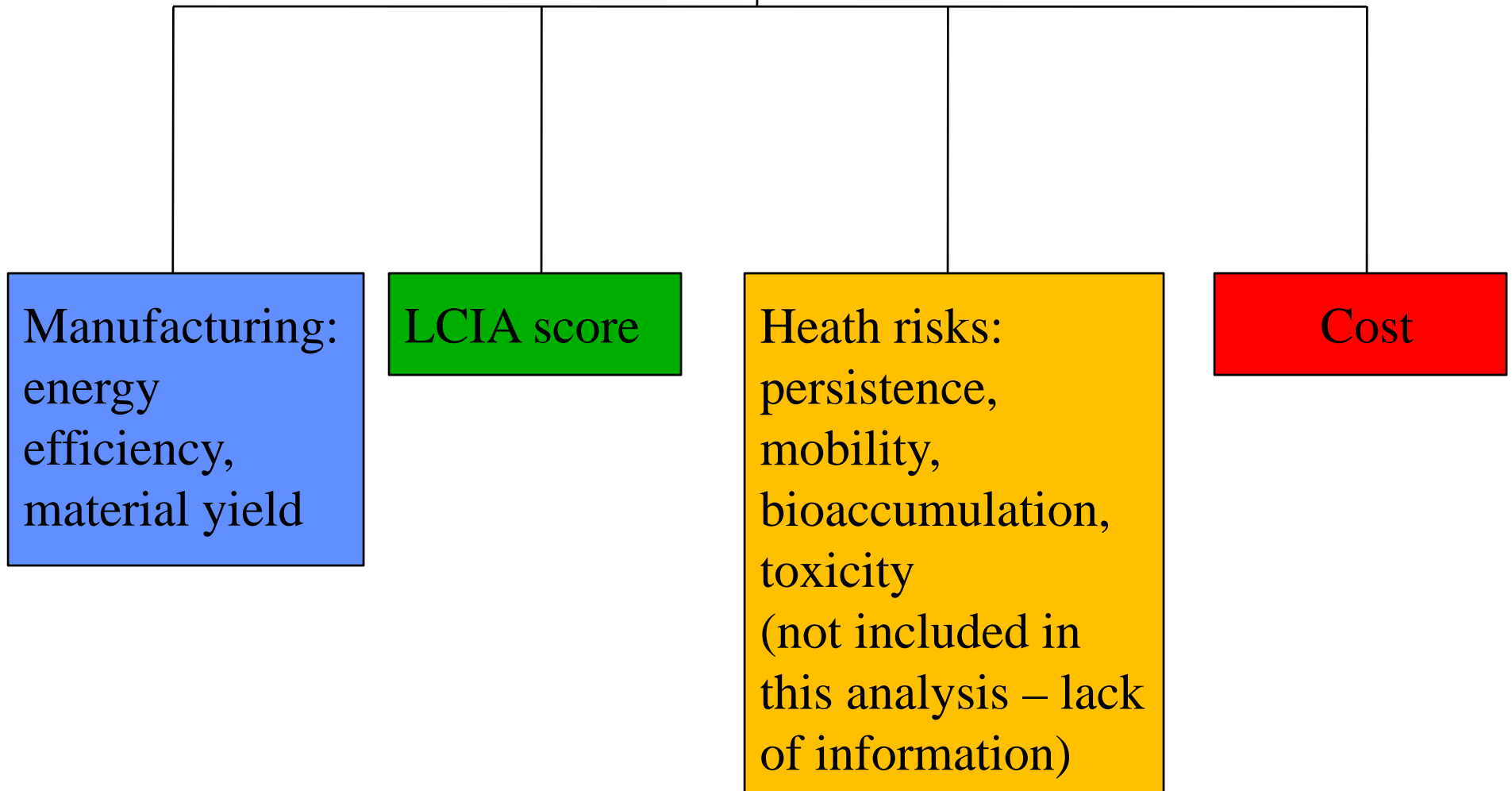*Based on Canis, Seager & Linkov (2010)*

A SCWNT-specific LCA: Manufacturing

Purposes of LCA:

- improvement assessment
- comparative decision-making

waste gas

CO_2

Carbon source & metal catalyst

energy

Argon gas

SYNTHESIS

PURIFICATION
acid wash, combustion

dissolved metals

waste acid

electrolyte

metals

Metal Electrode

Cut SWNT paper anode
Li+ Electrolyte
Celgard seperator
LiCoO₂
Copper foil support

Metal Electrode

e energy

charge energy

SWCNT photos provided by Brian Landi, Nanopower Research
Labs (Ryne Raffelle, Director) , Rochester Institute of Technology.

Criteria for the Comparison of Manufacturing Alternatives

Manufacturing: energy efficiency, material yield

LCIA score

Heath risks: persistence, mobility, bioaccumulation, toxicity (not included in this analysis – lack of information)

Cost

Material yield

■ RESEARCH AND ANALYSIS

## Environmental Assessment of Single-Walled Carbon Nanotube Processes

Meagan L. Healy, Lindsay J. Dahlben, and Jacqueline A. Isaacs

Table I Key yield parameters for production of single-walled nanotubes (SWNTs)

Process Parameter	Arc (%)	CVD (%)	HiPco (%)
Synthesis reaction yield (SRY)	4.50	2.95	0.08
Purification yield	70	90	90

Note: CVD = chemical vapor deposition; HiPco = high-pressure carbon monoxide.
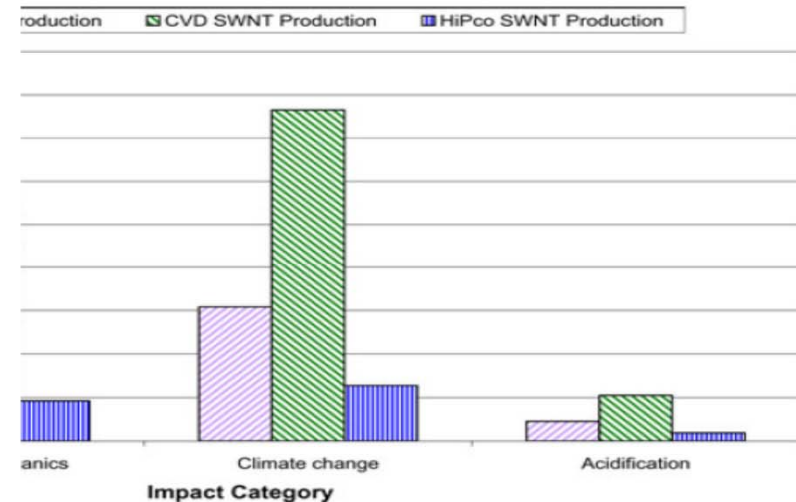
...position (CVD), and high-pressure carbon monoxide (HiPco) base case = single-walled nanotube; Pt = normalized impact per gram of product.
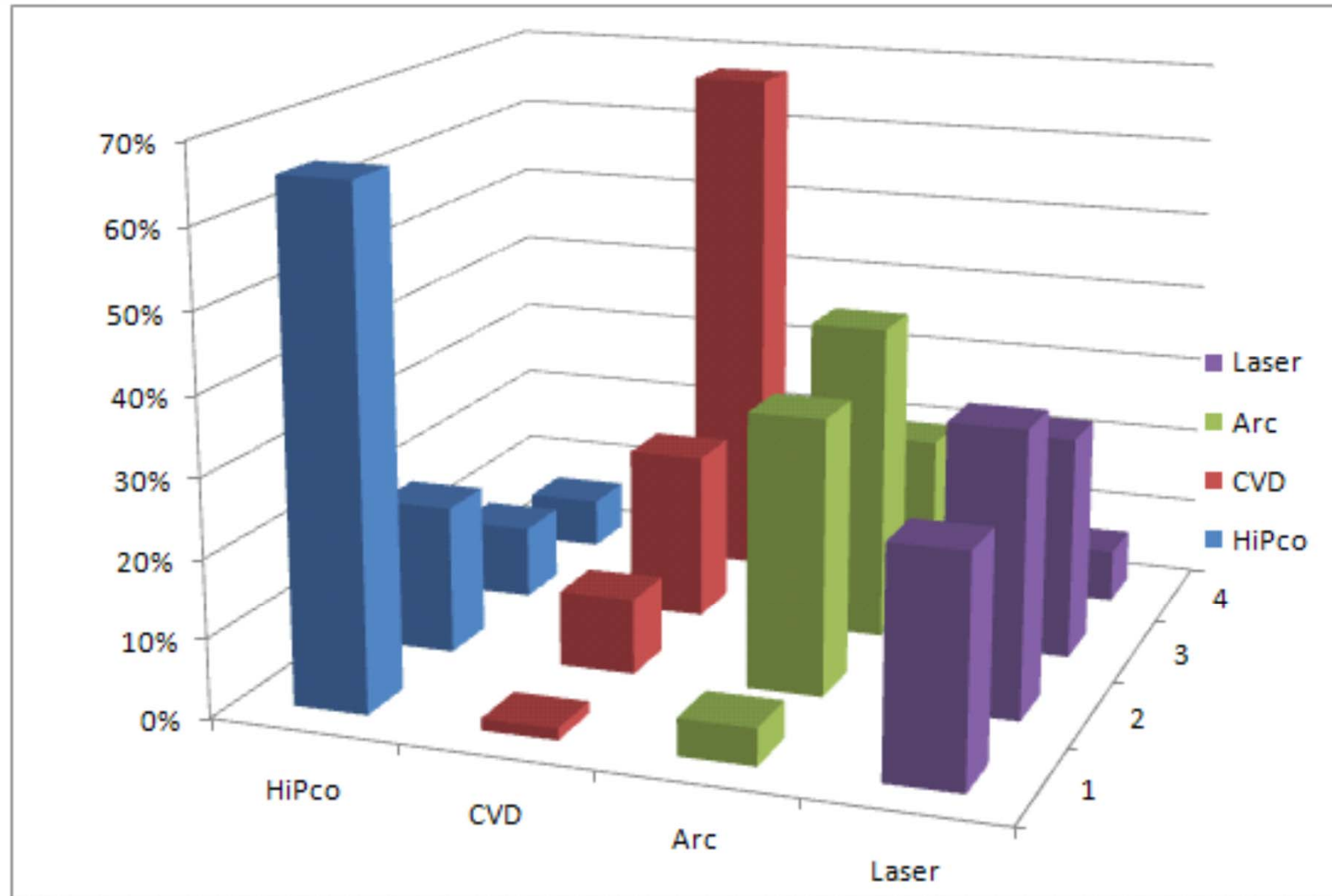
LCIA score

Literature Data represented as probability distributions or H, M, L

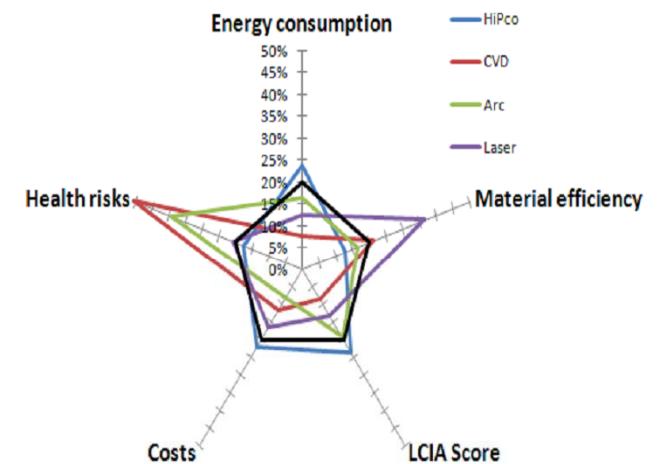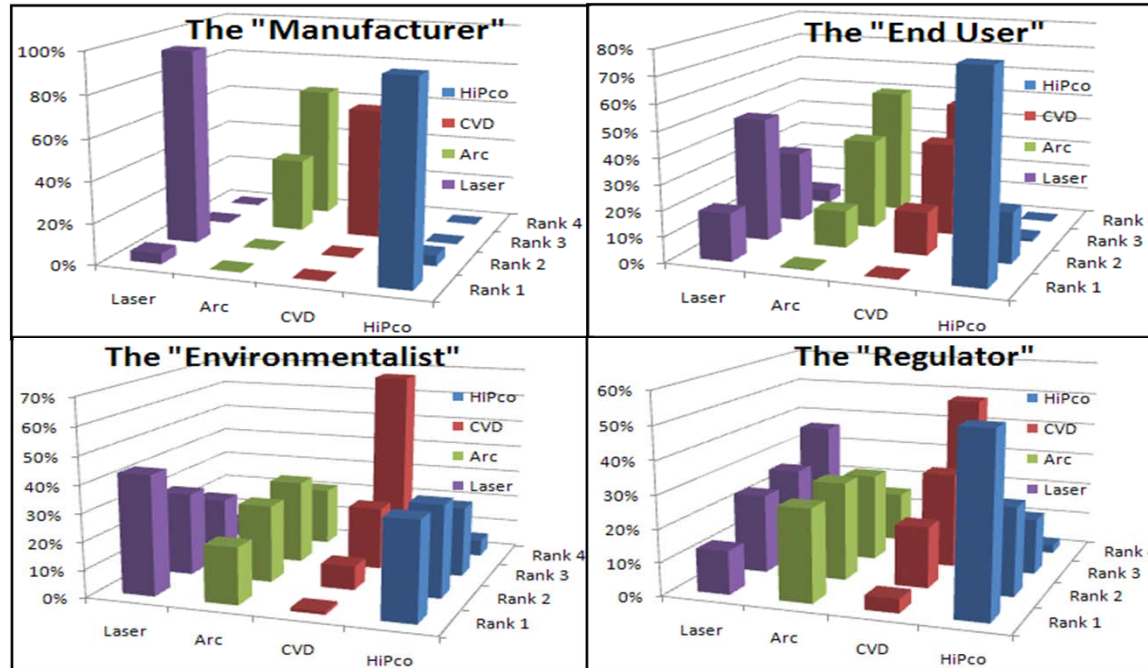| Alternative/ Criterion	Energy consumption (GWh/kg)	Material efficiency (% in mass)	LCIA Score (EcoPoints)	Cost ($/g)	Health risks
GOAL	Minimize	Maximize	Minimize	Minimize	Minimize
HiPco	0.05 0.21 0.36	0.00 0.23 0.45	1.48 20.69 39.90	242.50 1550.75 2859.00	L M H
CVD	0.05 0.21 0.36	0.00 0.23 0.45	1.48 20.69 39.90	242.50 1550.75 2859.00	L M H
Arc	0.05 0.21 0.36	0.00 0.23 0.45	1.48 20.69 39.90	242.50 1550.75 2859.00	L M H
Laser	0.05 0.21 0.36	0.00 0.23 0.45	1.48 20.69 39.90	242.50 1550.75 2859.00	L M H

Accounting for Stakeholder Preferences

- Sets of weights (or weight ranges) corresponding to different stakeholders can be established
  e.g., LCIA score is likely to be less important to manufacturers

- For each fixed set of weights, analysis can be run again

- For each stakeholder, we can obtain a relative ranking of manufacturing alternatives

- 5 risk categories
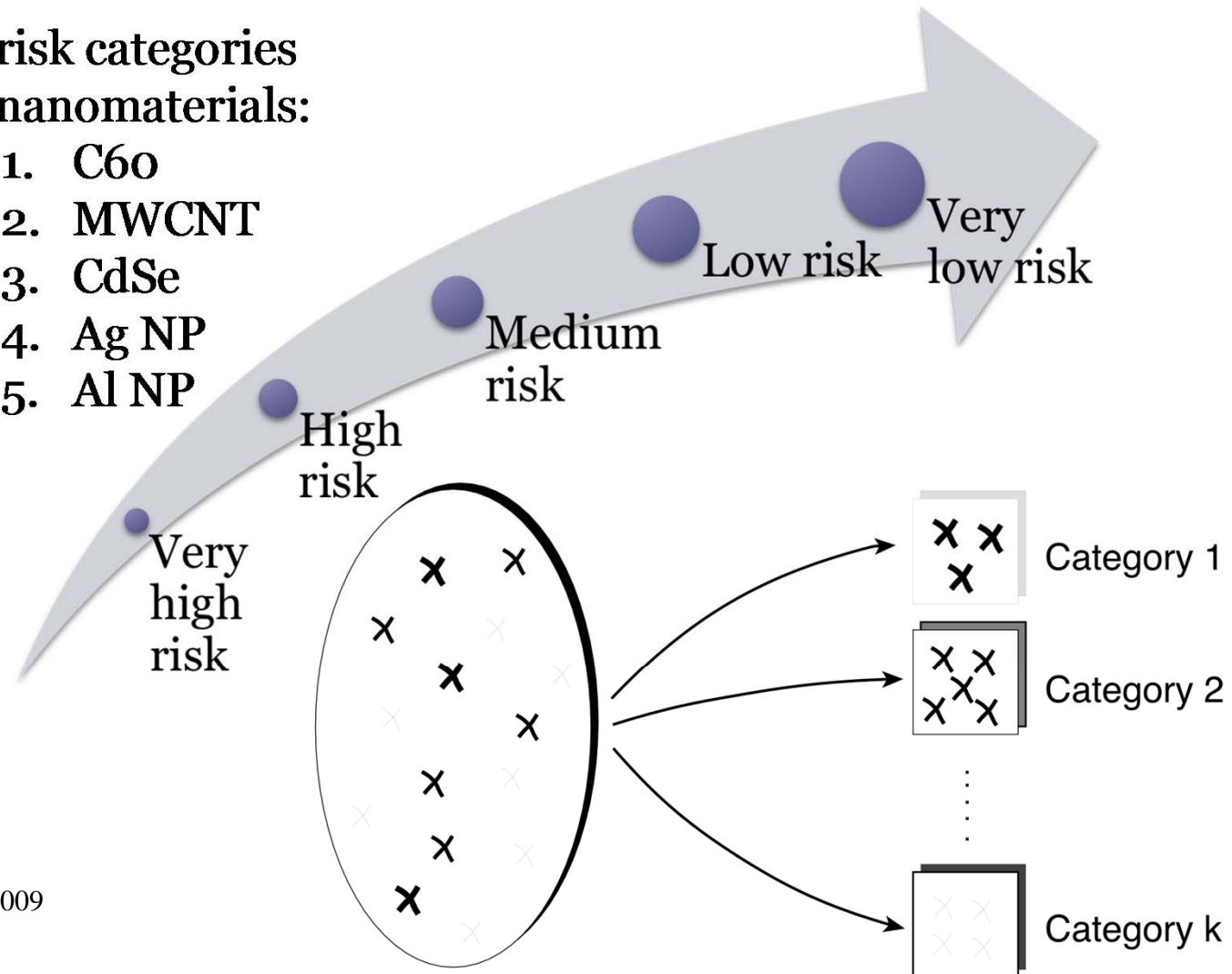- 5 nanomaterials:
  1. C60
  2. MWCNT
  3. CdSe
  4. Ag NP
  5. Al NP

Very low risk

Low risk

Medium risk

High risk

Very high risk

Category 1

Category 2

Category k

After Tervonen et al., 2009

Criteria Measurements

|	Agglomeration	Reactivity /charge	Crit. Function groups	Contaminant Dissociation	Bioavailability pot. (±10)	Bioaccumulation pot. (±10)	Toxic pot. (±10)	Size (±10%)
C60	4	2, 3	3	2	25	50	10	100
MWCNT	4	2, 3	4	3	25	50	25	50
CdSe	4	4, 5	1	4	50	75	75	20
Ag NP	3	4, 5	1	4	50	75	75	50
Al NP	5	1, 2	1	1	25	75	10	50

Risk Profiles

Profile	Agglomeration	Reactivity /charge	Crit. Function groups	Contaminant Dissociation	Bioavailability potential	Bioaccumulation pot.	Toxic pot.	Size
Extreme-high	4	4	4	4	100	100	100	5
High-medium	3	3	3	3	80	80	80	50
Medium-low	2	2	2	2	70	70	70	100
Low-very low	1	1	1	1	60	60	60	200
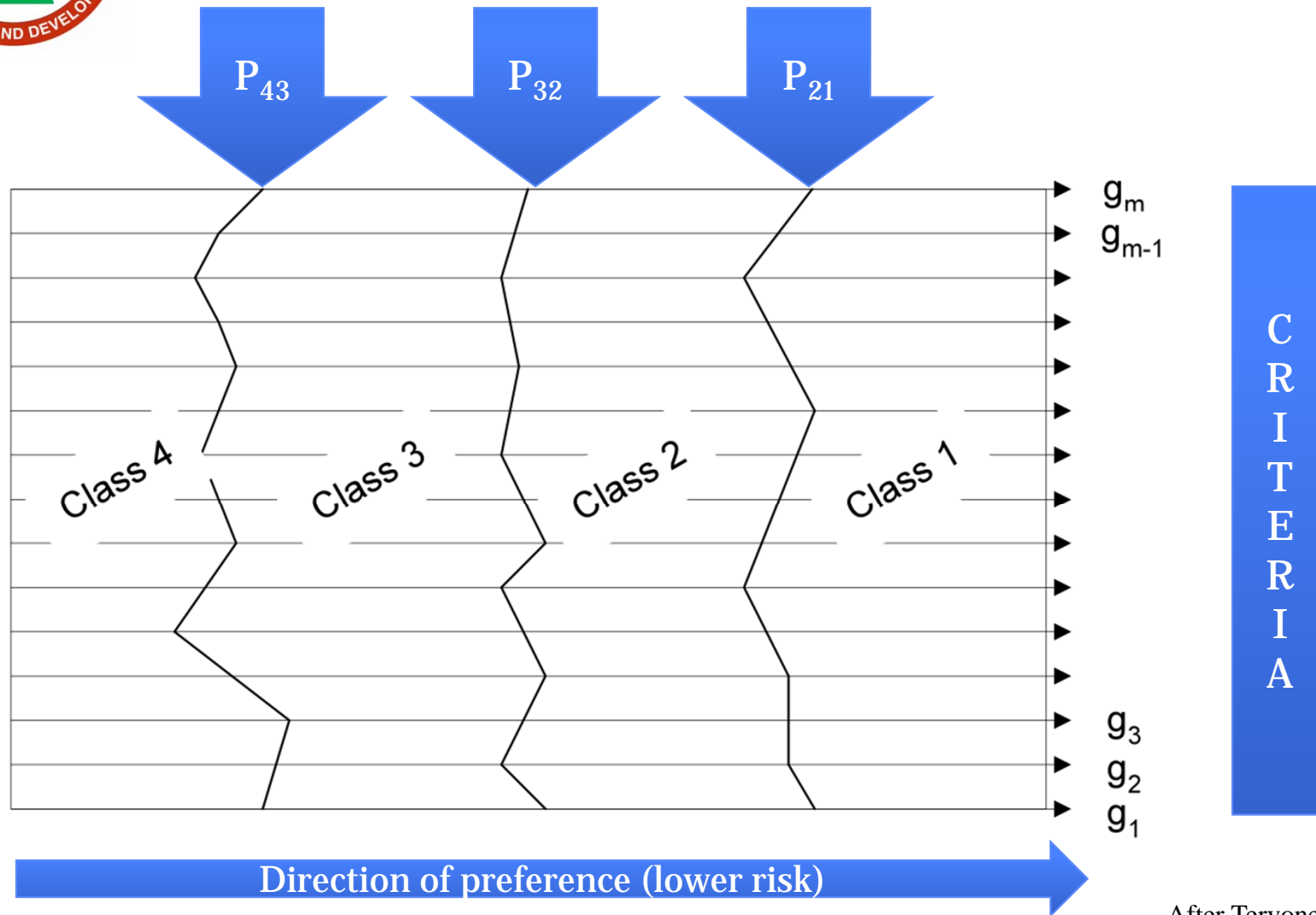
After Tervonen et al., 2009

Risk Classes

After Tervonen et al., 2009

	Extreme risk	High risk	Medium risk	Low risk	Very low risk
C60	0	0	51	49	0
MWCNT	0	26	73	1	0
CdSe	0	98	1	1	0
Ag NP	0	29	71	1	0
Al NP	0	0	33	34	34
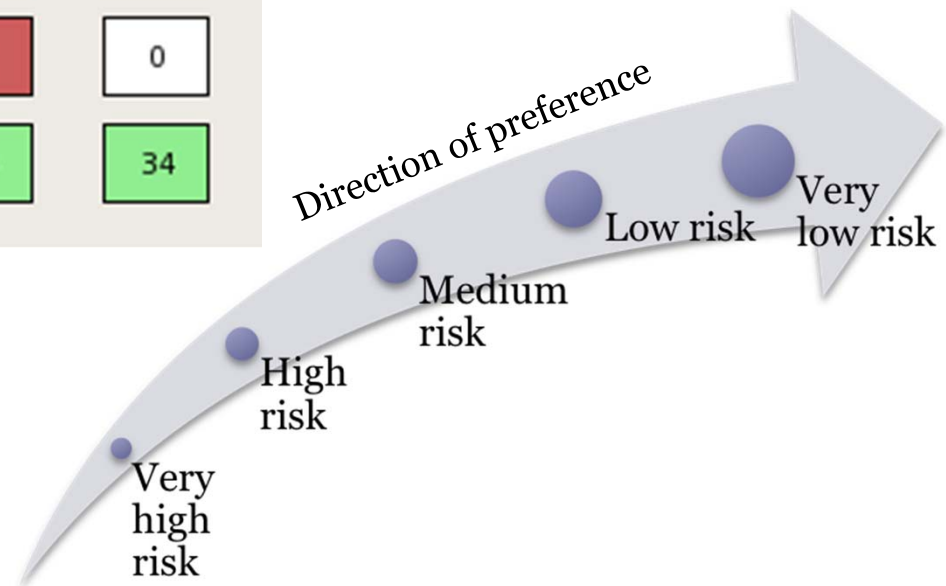
After Tervonen et al., 2009

How to Prioritize Research in the Context of This Specific Decision

- Research is only useful if it helps support and influence future decisions

- Is more precise information on health criteria useful? And on manufacturing criteria?

- What must be the quality of information for it to be useful?

- Are the benefits of additional information worth the costs?

# *What is Value of Information (VoI) ?*

- A measure of the value that information can bring in a decision context
    - Without information: the outcome of decisions are uncertain; the optimal decision yields a prior expected value
    - With information, the optimal decision can be made depending on the results; uncertainty is reduced; for each result, the optimal decision yields a posterior expected value; the total posterior expected value is their average
    - VoI: the difference between posterior expected value and prior expected value
- Computing VoI requires a decision model that can make the link between information and decisions
- Information is valuable if and only if it might switch the decision

| Net Flow of Best Alternative	No New Information	Manufacturing only	Health only	Full, Perfect Information	% of VoI from M Only	% of VoI from H Only
Manufacturer	63%	66%	63%	66%	100%	0%
Consumer	58%	58%	62%	63%	18%	84%
Regulator	38%	40%	56%	58%	9%	90%
Environmentalist	16%	16%	35%	35%	4%	99%
Balanced Weights	38%	39%	39%	41%	27%	48%
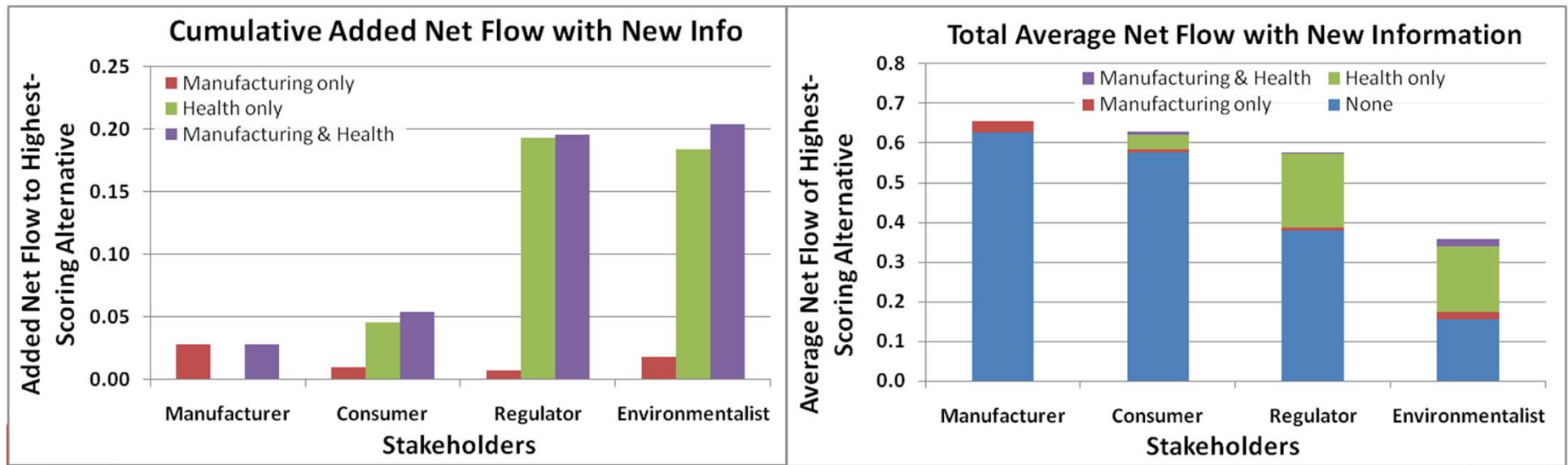
Total Average Net Flow with New Information
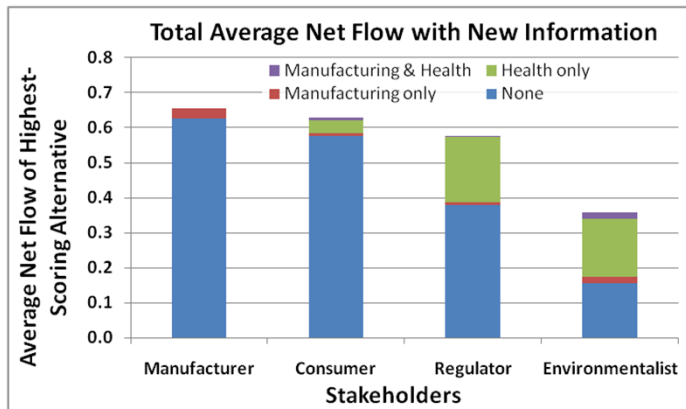
- Manufacturer & Consumer will be confident with their decisions

- Environmentalist & Regulator cannot decide with confidence

- Perhaps decision makers can make concessions to wary stakeholders

- Investing in health research will have the most impact

Cumulative Added Net Flow with New Info
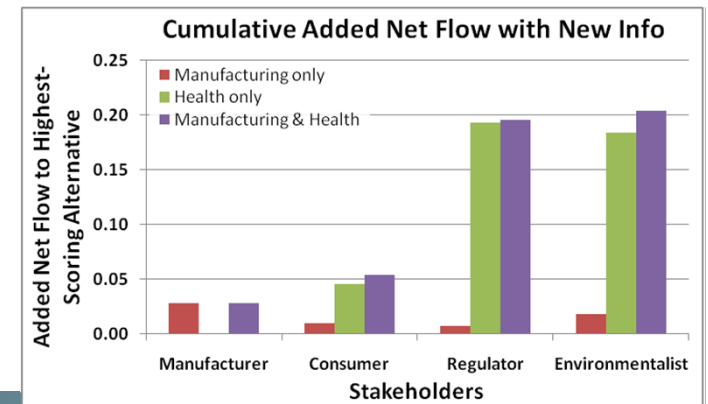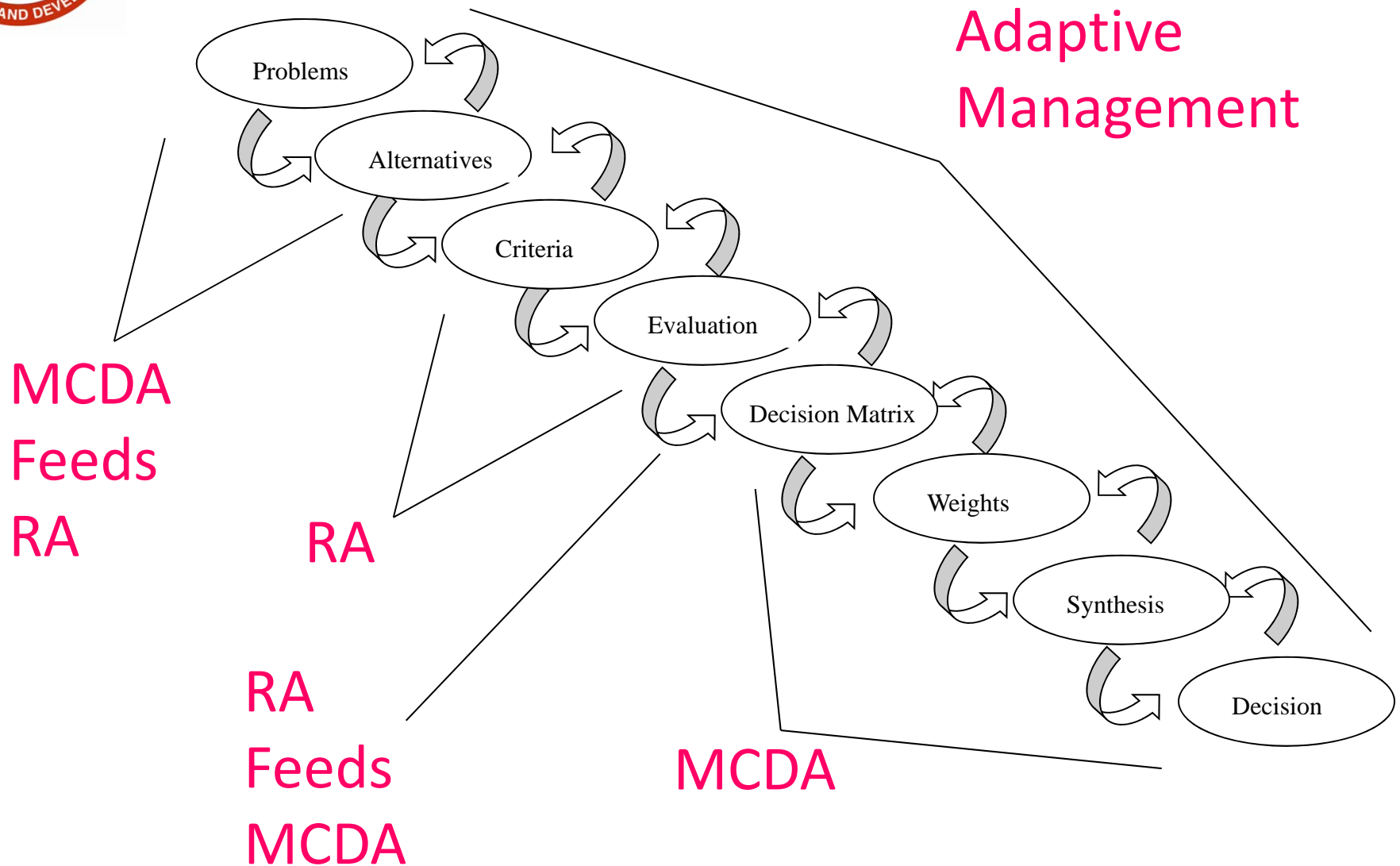
Summary: Essential Decision Ingredients

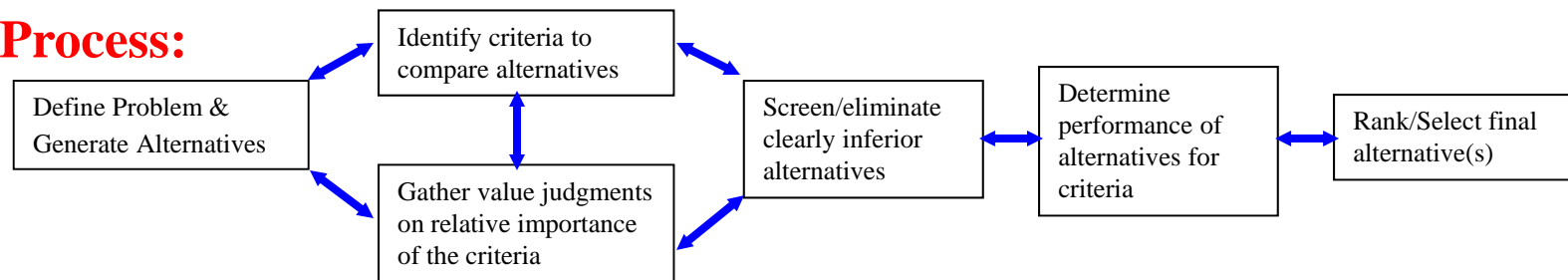**People**:

Policy Decision Maker(s)

Scientists and Engineers

Stakeholders (Public, Business, Interest groups)

Process:

Define Problem & Generate Alternatives → Identify criteria to compare alternatives / Gather value judgments on relative importance of the criteria → Screen/eliminate clearly inferior alternatives ↔ Determine performance of alternatives for criteria ↔ Rank/Select final alternative(s)

Tools:

Environmental Assessment/Modeling (Risk/Ecological/Environmental Assessment and Simulation Models)

Decision Analysis (Group Decision Making Techniques/Decision Methodologies and Software)

- There are clear benefits to be gained by advancing the use of formal risk and decision analysis methods:
  - Opportunities to explore trade-offs among diverse objectives
  - The ability to distinguish science and engineering inputs to a decision from values associated with objectives
  - Means for exploring the implications of uncertainty and the value of reducing it
  - Providing a quantitative framework to implement adaptive management

- However, efforts to apply these approaches will confront a number of practical issues related to the following:
  - Under-estimating the level of effort required to accomplish effective deliberation through the use of decision analysis
  - Determining who can/should be involved in value/preference elicitation
  - Intolerance for transparency in decision-making
  - The misconception that decision analysis is a substitute for an actual decision

- Decision models and Value of Information analyses can prove useful tools to:
    - Help making decisions under uncertainty
    - Assess whether information gathering has value in this context
- To help assess nanomaterials research options:
    - Several decision situations should be identified where information obtained from the research might be useful
    - A VoI analysis applied to these decision models coupled with an estimation of the costs of the research and the cost of delaying the decisions would help assess whether research proposals are worth the investment/ which ones are most worthy

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